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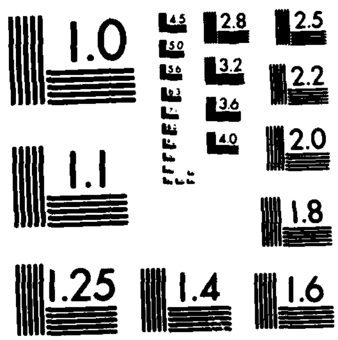

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Progress and results on four major areas is reported:

(i) Problems relating to correlations affecting the average field in a strongly coupled plasma;

(ii) Problems relating to the dispersion of plasma oscillations affecting the the fluctuating field in a strongly coupled plasma;

(iii) Analysis and establishment of methods for the calculation of the degree of ionization and of the shift of energy levels of an ion embedded in a strongly coupled plasma; and

(iv) Investigation of the dynamical fluctuating field in a strongly coupled plasm

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I. BACKGROUND

The purpose of the research work conducted under the Grant 81-0091 was to investigate the effect of a plasma environment on atomic and ionic bound states. This problem has many aspects, which can be classified as follows:

a) The effect of the average field on the position of energy levels.

b) The effect of the slow ionic fluctuations on the broadening of and merging of energy levels.

c) The effect of the rapidly fluctuating electronic field on the energy levels.

d) The self consistent determination of the degree of ionization in the system.

e) The determination of the spectrum and level of the fluctuating electric field acting on the bound states.

f) The self-consistent treatment of the electron-electron, electron-ion and ion-ion correlations affecting the average field.

g) Determination of the spectrum of plasma oscillations affecting the fluctuating field.

The complexity of the basic many body problem is compounded by the fact that plasmas of interest are of substantially high denisty ($n = 10^{19} \sim 10^{26}$ cm^{-3}) and contain high Z ($10^{\sim 17}$) atoms of high degree of ionization: these circumstances render the ambient plasma strongly coupled, a situation that will be discussed below.

Strong coupling arises when the (potential energy)/(kinetic energy) ratio is of the order of or exceeds unity. The relevant parameters are:

$$\Gamma = \frac{Z^2 e^2}{dkT} \qquad \text{or} \qquad \gamma = \frac{\kappa^2}{4\pi n}$$

with d being the interpartide distance and κ the inverse Debye length; strong coupling means $\Gamma > 1$ or $\gamma > 1$. In the systems of interest $\gamma = 1 \sim 20$. For this reason, conventional perturbation approaches do not work in such systems. Our earlier work,[1,2] done mostly under AFOSR Grant 76-2960, had established a framework for the treatment of strongly coupled plasmas. Application of these earlier developed methods in the context of the problems posed by the present Grant was a part of the research performed.

The domain of applications of the problem of strongly coupled plasma - bound state interaction is laser or particle beam compressed plasmas and plasma media for X-ray lasers. Our work was done primarily with the second objective in mind, but it didn't reach the stage where concrete application could have been worked out.

II. RESEARCH WORK

Our research work concentrated in four general areas.

(i) Problems relating to correlations affecting the average field in a strongly coupled plasma.

(ii) Problems relating to the dispersion of plasma oscillations affecting the fluctuating field in a strongly coupled plasma.

(iii) Analysis and establishment of methods for the calculation of the degree of ionization and of the shift of energy levels of an ion embedded in a strongly coupled plasma.

(iv) Investigation of the dynamical fluctuating field in a strongly coupled plasma.

Discussion of these items now follows:

(i) The description of correlations in two- or multi-component strongly coupled plasmas requires generalization of the methods already developed by us[1] for one-component systems. This has been undertaken in a number of publications. Even though there are no bound systems (atoms or ions) in this model, the analysis of the formalism is a a necessary prerequisite of the description of media with bound systems. In Publication A we analyzed the cornerstones of our approximation scheme, the VAA (Velocity Average Approximation) and the NLFDT (Non-Linear Fluctuation-Dissipation Theorem).

A convenient method to analyze the kinetics of strongly coupled plasmas is by way of partial response functions. This method was originally suggested by Singwi and Vashista[3] and then further analyzed and extended by Golden and Kalman[4]. However, attempts to use this approach for concrete calculations have been frustrated by the apparent complexity and unwieldiness of the formalism. We have succeeded to cast the formalism in a much simpler language by using matrix description in "species-space". By exploiting this new formalism we have obtained some new and important results: (a) we have found that at least one of the ion-ion pair correlation functions in a multi-ion system exhibits an oscillatory behavior for arbitrary small coupling; (b) we have shown that if quantum and proximity corrections are taken into account in the interaction potential -which make the A-B interaction different from the A-A interaction (apart from scale), -the dielectric function exhibits a qualitatively new behavior; (c) by examining the structural features of the well-known Totsuji-Ichimaru approximation scheme for multi-species systems, we have discovered that it violates an important symmetry requirement and therefore its applicability to multi-species systems is doubtful.

These results were the outcomes of a major paper addressing itself primarily to the basic formalism (Publication B); further papers on the details of results listed above are Publications D and E.

Another aspect of our research is based on an approximation scheme (the Golden-Kalman (GK) approach)[1] which combines the plasma kinetic equations with nonlinear fluctuation-dissipation relations. The physical transparency and mathematical tractability of the resulting chain of response function equations, which had already provided a very good qualitative description of one-component plasma collective modes in the strong coupling regime[2], led us to believe that the GK procedure will be equally effective in the treatment of the corresponding multi-component plasma problem. Until recently, the needed fluctuation-dissipation relations had been lacking. These relations have been established by us for both binary ionic mixtures and fully ionized ion-electron plasmas. Our principal frequency domain result links a single three-point dynamical structure function to a combination of nonlinear partial response functions. These results are given in Publication C.

(ii) Works listed under (F) and (G) deal with the problem of plasma oscillations in strongly coupled systems. Plasma oscillations are expected to reach a high level of excitation ($\sim\gamma$) for strong coupling. The ensuing dynamical perturbation on the bound states becomes substantial and the knowledge and understanding of the percise plasmon spectrum under these circumstances is essential. Publication F analyzes the relationship between perturbation theoretic and the non-perturbative GK approach. This latter method was applied some time ago[2] to the problem of plasmon dispersion and gave very good agreement with molecular dynamics computer simulations[4] as far as the plasmon dispersion was concerned, but the agreement with the width of the plasmon peak was rather poor. An improvement of our original approach described in (G) now has provided a remarkably good agreement in this connection as well, including the reproduction of the non-monotonic γ-dependence of the width. To the best of our knowledge this the first successful theoretic description of this unexpected behavior.

An earlier work (Publication 4) done while the authors were Research Leaders at the International Centre for Theoretical Physics, Trieste clarifies a controversial aspect about the slope of plasmon dispersion curve for strong coupling - an issue which can have important consequences for laser scatterings experiments. A further item of clarification was provided in Publication I on the physical relationship between linear and nonlinear response functions whose interrelatedness plays a central role in our dynamical approximation scheme. Finally, in this group, a number of invited review talks and lecture series were given at various national and international meetings (N,P,Q,R,S,T,U,V).

(iii) There are a number of methods available for the study of the dynamics of an atom or ion immersed in an ionized medium[5]. The Thomas-Fermi (TF) method combines relative simplicity with excellent qualitative descriptive capability. While the TF scheme and its refinement have been employed to the problem on hand, the approaches used are appropriate for weakly coupled situations and not for the case of strong coupling. The scheme we have worked out is intended to include specific strong coupling effects and is summarized below.

- The system is considered to consist, for the purpose of the TF equation, of three species:
  - (i) N_i classical nuclei of charge Z,
  - (ii) $N_e = N_i X$ hot, classical, "free" electrons, and
  - (iii) $N_b = N_i Y$ ($Y=Z-X$) degenerate bound electrons.
- The potential around a chosen nucleus is determined by the Poisson-equation with the g_{ei} and g_{ii} pair correlation functions providing the density distribution of the surrounding particles.

- For the purpose of the calculation of the correlation functions the system consists of
  - (i) N_i ions of charge X and
  - (ii) N_e hot classical, "free" electrons, interacting through the effective potentials Φ_{ee}, Φ_{ii} and Φ_{ei}, such that $Z > Z_{eff} > X$.
- $Z_{eff,\ i}$ and $Z_{eff,\ e}$ are to be determined by the integrated charge densities of the bound electrons only.
- The correlation functions g_{ee} and g_{ei} are now to be determined by using one of the strongly coupled static plasma schemes-either the mean field theories, or HNC.
- Finally X is to be determined by calculating the free energy of the system and minimizing it with respect to X.

The salient feature of this scheme is that it applies the philosophy of the TF-DH (Debye-Huckel) method, but replaces the DH distribution with the correlation functions appropriate for strong coupling. In turn, the correlation functions depend on the effective potentials. The splitting of the population into "classical" and "bound" electrons allows one to take into account electron-electron and electron-ion correlations: should one treat the entire electron population in the framework the original TF scheme, the inclusion of correlations would be an almost insurmountably difficult task.

Based on a survey of the earlier TF and TF-DH works, starting with the early works of Feynman, Metropolis and Teller[6] and Latter[6] through the more recent works of Rozsnyai and Alder[7] and More and Skupsky[8], the superiority of our scheme, as outlined, over the existing approaches is quite convincing.

One of the principal features of the model described above is that the plasma particles are considered interacting through an effective potential which is different from the bare Coulomb potential because of the screening effect of the bound electrons and which is species dependent, i.e. is different for electron-electron, electron-ion and ion-ion interactions. The strong correlations between the particles are taken into account via a mean field theory (MFT)[9]. While, however, the various MFT-s have been studied in great detail for the simplified one component plasma model, the formal structure of the MFT for the situation of interest had to be established. We accomplished this in the already quoted Publication (B) in which the partial response function formalism, cast in a matrix language was used to set up the frame for the calculations.

The precise degree of ionization in a dense plasma is one of the most difficult questions to answer. The scheme described above is expected to provide a value for the degree of ionization X; however, for the purpose of comparison we have also pursued an independent approach to the problem, through the standard method of Saha-equation. However, the Saha-equation, based on a model of a gas composed of independent particles, becomes quite unreliable at high densities. The main effects ignored by the Saha-equation treatment are (i) the proximity effect, and (ii) the depression of the ionization potential, which itself consists of the depression of the continuum and of the lifting of the bound states due to screening. In Publication J we have developed and analyzed a model which shows the effect of the latter. The influence of the medium on the atom is described through the replacement if the intra-atomic potential by a screened Debye-potential where the screening constant $\kappa = (4\pi e^2 n\beta)^{1/2}$

depends on the free electron density. Increasing values of κ cause the disappearance of high-lying bound states, leading to the elimination of the last bound state at $\kappa a \simeq 1.1$ (a = Bohr-radius)[10]. Consequently, ionization becomes easier, and the calculated degree of ionization is substantially above the simple Saha result. Moreover, as more electrons become free, the ionization potential is further depressed and an avalanche develops generating a sudden phase-transition-like from the weakly ionized to a highly ionized state. We have used the recent analytic approximation given by Green[11] to describe the bound states in a screened potential. The Saha-equation was modified by using the Larkin correction[5] for the partion function. The resulting rather complex self-consistency condition for the degree of ionization was solved numerically. Detailed computer work has been performed recently with parameters pertaining to H-plasmas in a wide range of densities, up to the degeneracy limit. We have found the phase-diagram in the density-temperature plane, with a critical point in the vicinity of $T_c = 3$ eV, $n_c = 3 \times 10^{23}$ cm^{-3}.

(IV) The high level of plasma oscillations in the strong coupling regime provides a high-frequency (dynamic) electric field, acting on the atomic level structure and affecting the ensuing radiation. For a plasma in thermal equilibrium, the magnitude of these oscillations can be expected to be rather small for weak coupling, but the situation changes for strongly coupled plasmas, and both the static (Holtsmark) and dynamic (electronic) fields must be taken into consideration for their effects on energy levels and line broadening.

In Publications K,L,M we addressed the question of the strength of these dynamical field oscillations in strongly coupled plasmas. Employing the structure factors obtained by Molecular Dynamics (MD)[12] experiments, we assessed the strength and dispersion characteristics of the plasma dynamical fields. The main result can be represented in terms of the electron coupling parameter $\Gamma = e^2/aT_e$ as

$$W_d/nT = \begin{cases} (3\Gamma)^{3/2}/9\pi, & \Gamma \ll 1 \\ q_{max}^3/9\pi, & \Gamma \gtrsim 1 \end{cases}$$

where W_d is the energy density for the dynamical oscillations, $q = ka$, and a is the electron sphere radius. q_{max} can attain values ≈ 2 for $\Gamma > 10$, allowing a significant fraction of energy to reside in the dynamical oscillations.

For typical high density plasmas, the level splitting of the 2p 2s state due to the self consistent potential for $Z - 10$, $T_e \approx 1$keV and $n_e = 5 \times 10^{24}$ cm^{-3} is 5 eV. The corresponding ionic Stark effect is $\approx$ 6 eV, and the dynamical field strength has the value $\approx$ 4 eV, and the dynamical frequency, expressed in energy units is $\approx$ 80 eV.

This serves as a reference point, and the fields and frequency at other densities and temperatures can be obtained through the scalings:

Dynamical Field $E_D \sim (n_e T_e \gamma_e)^{1/2}, \sim n_e^{3/4} T_e^{-1/4}$

Dynamical frequency $w_p \sim n_e^{1/2}$

Static field $E_S \sim (n_e/Z)^{2/3}$

Degenerate level splitting $(\Delta E) \sim n_e/Te$ (Debye-Huckel potential)

or $\sim n_e/Z^2$ (Uniform electron screening)

Thus we can infer that the static and dynamical effects will "mix" for a wide variety of strongly coupled plasmas. The static field splitting and the degenerate-level splitting due to screening will remain comparable for density ranges $n_e \sim 10^{20}$ to 10^{24}, and temperatures $T_e \sim 50$ to 500 eV.

The important parameters for the interplay of dynamical and static field effects are $D \sim E_D/\omega p$ and $S \sim E_S/\omega_p$. The former scales as $n_e^{1/4}\ T_e^{-1/4}$ for $\gamma_e<1$, and this variation is not too severe over the range of interest. The latter scales as $n_e^{1/6}\ Z^{-2/3}$, and for fixed Z, the density related variation is quite mild.

We have also analyzed the time dependence of the dynamical field seen by an atom. When the spread in frequencies ω for the dynamical fields is negligible, (i.e. the dispersion in ωpeak due to the spread is k is negligible, as is the case, approximately for $\Gamma \sim 10$), all the dynamical components lead to a coherent oscillation at $\omega \approx \omega_p$. The individual micro-oscillations in any direction last only for a few periods, of the order of ω_p/γ, where the damping rate γ is proportional to $\Delta\omega$, the halfwidth of the peaked S(k, w). The rise and decay of individual microfields leads to an oscillation with a common frequency ω_p, but with a slowly wandering complex amplitude $E_d(t)$ on a time scale $1/\gamma$, much longer than the plasma period. Thus the atom essentially experiences an "external field" of magnitude $E_d = (8\pi W_d)^{1/2}$, albeit of complex polarization. The space dependence of the fields is irrelevant as long as the wavelengths are much larger than the atomic size.

From the point of view of the modifications of the atomic energy level structure, the slow wander in $E_d(t)$ one can ignore as a first approximation. The resultant spectral effects can be described by the Blokhintsev theory for a simple polarization. However, when the polarization is more complex, or quasi-static fields of comparable amplitude are also present, the more general theory of combined static and dynamic fields developed by us some time ago becomes necessary.

III. PUBLICATIONS AND PRESENTATIONS

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P. K.I. Golden: Lectures on Strongly Coupled Plasmas, Workshop on Condensed Matter, International Centre for Theoretical Physics, Trieste, Italy, August, 1981.

Q. G. Kalman: Nonlinear Response Functions and Collective Modes in a Strongly Coupled Plasma, lectures given at the Winter Workshop on the Statistical Mechanics of Ionic Matter, Les Houches, France, April 1982.

R. K.I. Golden: Lectures on Strongly Coupled Surface Plasmas, Workshop on Condensed Matter, International Centre for Theoretical Physics, Trieste, Italy, August 1983.

S. K.I. Golden, G. Kalman and De-Xin Lu: Nonlinear Fluctuation-Dissipation Theorem for Plasma Mixtures, invited paper presented at the Conference on Statistical Mechanics, Davis, CA, March 1984.

T. G. Kalman and K.I. Golden: Dynamical Theory of Strongly Coupled Plasmas, invited paper presented at the Conference on Statistical Mechanics, Davis, CA, March 1984.

U. G. Kalman: Plasma Oscillations in Strongly Coupled Bulk and Surface Plasmas, Memorial Workshop on Condensed Matter, International Centre for Theoretical Physics, Trieste, Italy, August 1984.

V. G. Kalman: Plasmon Dispersion in Strongly Coupled Plasmas, invited paper presented at the XIIth Symposium on the Physics of Ionized Gases, Sibenik Yugoslavia, September 1984; to appear in the Proceedings of the Symposium.

Dr. G. Kalman was invited lecturer at NATO Workshop on the Statistical Mechanics of Ionic Matter, Les Houches, April 1982; Dr. G. Kalman and Dr. K. Golden were invited lecturers and Research Leaders at the Workshop on Condensed Matter, Intenational Centre for Theoretical Physics, Trieste, August 1981. Dr. G. Kalman was invited lecturer at the NATO Workshop on the Statistical Mechanics of Ionic Matter, Les Houches, April 1982; Dr. K. Golden was invited lecturer at various institutions in the People's Republic of China, and at universities in Australia in the summer of 1982; Dr. G. Kalman was invited lecturer at the 2nd International Meeting on Non-Ideal Plasmas, Wustrow, DDR, October, 1982; Dr. G. Kalman was the convener of a session on strongly coupled plasmas on behalf of the Organizing Committee for the XVIth International Conference on Ionization Phenomena in Gases, August, 1983; Dr. K. Golden was invited lecturer and Research Leader at the

International Centre for Theoretical Physics, Trieste, August 1983; Dr. G. Kalman, Dr. K. Golden and Dr. P. Bakshi were invited lecturers at the Conference on Statistical Mechanics, Davis, CA, March 1984.

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IV. PERSONNEL

Dr. G. Kalman, Principal Investigator

Dr. K.I. Golden, Consultant

Dr. P. Bakshi, Senior Investigator -- (February 1, 1983 through January 31, 1984)

Dr. P. Carini, former graduate student. (Degree awarded: June, 1983)

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